Author Index to Volume 10

Adamowicz, L.
Coupled Cluster Method with First-Order Correlation Orbitals versus Multireference Configuration Interaction Method. Accurate Calculations for HF, H_2O, and NH_3, 928
Ahlrichs, R. See Häser, M., 104
Alcamí, M.
—; de Paz, J. L. G.; Yáñez, M.: Nitrogen Inversion Barriers in Three-Membered Rings. An *Ab Initio* Molecular Orbital Study, 468
Allinger, N. L. See Lii, J.-H., 503
—; See Tai, J. C., 635
Anderson, J. See Miller K. J., 63
Anvia, F. See Catalán, J., 426
Aped, P.
—; Schleifer, L.; Fuchs, B.; Wolfe, S.: Probing the Anomeric Effect. The Diaminomethylene Group: Calculations of *N—C—N*-Containing Molecular Systems, 265

Bachrach, S. M.
Topological Electron Density Analysis of Phosphines, Phosphaalkenes and Phosphaalkynes, 392
—; Streitwieser, A.: Application of Various Population Methods to Some Oxygenated Compounds, 514
Baeck, K. K. See Lee, Y. S., 112
Baker, B. See Lipkowitz, K. B., 718
Balasubramanian, K. See Hosoya, H., 698
—; See Liu, X., 1, 417
Bellido, M. N.
—; Rullmann, J. A. C.: Atomic Charge Models for Polypeptides Derived from *Ab Initio* Calculations, 479
Bender, C. See Lii, J.-H., 503
Biran, G. See Faegri, K., 495
Boulu, L. G.
—; Crippen, G. M.: Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy, 673
Boyd, R. J.
—; Wang, L.-C.: The Effect of Electron Correlation on the Topological and Atomic Properties of the Electron Density Distributions of Molecules, 367
Braga, J. P.
The Rate of Convergence of the S Matrix for the Renormalized Numerov and Log-Derivative Methods, 413
Bunce, J. D. See Venanzi, C. A., 1038

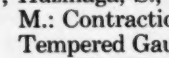
Canzius, P. M. See Venanzi, C. A., 1038
Cao, X.
Molecular Symmetry and *Ab Initio* Calculations. I. Symmetry-Matrix and Symmetry-Supermatrix, 957
Carballeira, L.
—; Mosquera, R. A.; Rios, M. A.: Molecular Mechanics of Peroxides. II. Cyclic Compounds, 911
Cartledge, F. K. See Cho, S. G., 832
—; See Profeta, S., Jr., 99
Catalán, J.
—; Sánchez-Cabezudo, M.; de Paz, J. L. G.; Elguero, J.; Taft, R. W.; Anvia, F.: The Tautomerism of 1,2,3-Triazole, 3(5)-Methylpyrazole and Their Cations, 426
Chang, D. K.
—; Urry, D. W.: Polypentapeptide of Elastin: Damping of Internal Chain Dynamics on Extension, 850
Chen, R. S.
Monte Carlo Simulations for the Study of Hemoglobin-Fragment Conformations, 488
Chesnut, D. B.
—; Moore, K. D.: Locally Dense Basis Sets for Chemical Shift Calculations, 648
Cho, S. G.
—; Unwalla, R. J.; Cartledge, F. K.; Profeta, S., Jr.: Chlorosilanes: Development and Application of MM2 Force Field Parameters, 832
Choi, J. Y.
—; Davidson, E. R.; Lee, I.: AM1 Studies on the Potential Energy Surface for the Proton Transfer in Protonated Water Clusters, $H^+(H_2O)_n$, 163
Chung-Phillips, A.
Deorthogonalization of Atomic Orbitals in the CNDO Approach, 17
—; Methods for the Fourier-Series Expansion of Torsional Energies, 733
Clark, M.
—; Cramer R. D., III; Van Opdenbosch, N.: Validation of the General Purpose Tripos 5.2 Force Field, 982
Cramer, R. D., III See Clark, M., 982
Crippen, G. M.
Linearized Embedding: A New Metric Matrix Algorithm for Calculating Molecular Conformations Subject to Geometric Constraints, 896
—; See Boulu, L. G., 673
Cummins, P. L.
—; Gready, J. E.: Computational Strategies for the Optimization of Equilibrium Geometries and Transition-State Structures at the Semiempirical Level, 939

Dagher, M. See Kobeissi, H., 358
Dai, B. See Gimarc, B. M., 14
Dammkoehler, R. A. See Labanowski, J. K., 1016
Darden, T.
A Method for Fitting a Smooth Ribbon to Curved DNA, 529
Davidson, E. R. See Choi, J. Y., 163
Davis, M. E.
—; McCammon, J. A.: Solving the Finite Difference Linearized Poisson-Boltzmann Equation: A Comparison of Relaxation and Conjugate Gradient Methods, 386
de Gale, D. See Jain, D. C., 1031
de Paz, J. L. G. See Alcamí, M., 468
—; See Catalán, J., 426
Del Bene, J. E.
An *Ab Initio* Molecular Orbital Study of the Structures and Energies of Neutral and Charged Bimolecular Complexes of NH_3 with the

Hydrides AH_n (A = N, O, F, P, S, and Cl), 603
Diez, E. See Esteban, A. L., 887
Dingle, T. W.
—; Huzinaga, S.; Klobukowski, M.: Contraction of the Well-Tempered Gaussian Basis Sets: The First-Row Diatomic Molecules, 753
Du Toit, L. See Saldanha, J. W., 975

Ehrenson, S.
Continuum Radial Dielectric Functions for Ion and Dipole Solution Systems, 77
El-Hajj, A. See Kobeissi, H., 358
Elber, R. See Yip, V., 921
Elguero, J. See Catalán, J., 426
Eliel, E. L. See Olefirowicz, E. M., 407
Esteban, A. L.
—; Galache, M. P.; Mora, F.; Diez, E.; San Fabian, J. : Long-Range Proton-Proton Coupling Constants. I. Propanic Coupling Involving a Methyl Group $^4J_{MeH}$, 887
Eyraud, V. See Karfunkel, H. R., 628

Faegri, K., Jr.
—; Biran, G.: Basis Set Quality versus Size II. Approximate GTO Wave Functions for Second Row Transition Metal Atoms, 495
Fărcaşiu, D.
—; Walter, P.; Sheils, K.: Calculation of Number and Free Energy of the Conformers of Linear Alkanes with Medium and Long Chains. Implications for Catalysis, 520
Fasold, E. See Jug, K., 965
Ferguson, D. M.
—; Glauser, W. A.; Raber, D. J.: Molecular Mechanics Conformational Analysis of Cyclononane Using the RIPS Method and Comparison with Quantum-Mechanical Calculations, 903
Flores, J. R. See Redondo, P., 295
Floris, F.
—; Tomasi, J.: Evaluation of the Dispersion Contribution to the Solvation Energy. A Simple Computational Model in the Continuum Approximation, 616
Flurchick, K. M. See Lii, J.-H., 503

Ford, G. P.
—; Smith, C. T.: An MNDO Molecular Orbital Study of the Reactions of Protonated Oxirane Derivatives

($HCHCH_2OH^+$, X = CN, Cl, CH_3, Ph) with Simple Nucleophiles. Implications for Regioselectivity in the Reactions of Electrophiles with Nucleic Acid Bases, 568
François, J.-P. See Voets, R., 449
—; See Martin, J. M. L., 152, 346, 875
Fuchs, B. See Aped, P., 265
Fujita, T. See Sotomatsu, T., 94

Galache, M. P. See Esteban, A. L., 887
Gallion, S. See Lii, J.-H., 503
Garmer, D. R.
Extrapolation of the Time-Step Bias in Diffusion Quantum Monte Carlo by a Differential Sampling Technique, 176
Geise, H. J. See Van Alsenoy, C., 302
Gerig, J. T. See Gregory, D. H., 711
Gijbels, R. See Martin, J. M. L., 152, 346, 875
Gimarc, B. M.
—; Dai, B.; Ott, J. J.: *Ab Initio* SCF MO Results for the Carborane Isomers 3,5-$C_2B_6H_8$, 1,7-$C_2B_7H_9$, and 1,2-$C_2B_7H_9$, 14
Glaser, R.
The Density Integration Approach to Populations. A Critical Comparison of Projection Populations to Populations Defined by the Theory of Atoms in Molecules, 118
Glauser, W. A. See Ferguson, D. M., 903
Gō, N. See Higo, J., 376
Gopinathan, M. S. See Jug, K., 965
Gready, J. E. See Cummins, P. L., 939
—; See Jordan, M. J., 186
—; See Williams, M. L., 35
Gregory, D. H.
—; Gerig, J. T.: Force Field Parameterization for the 4-Fluorophenyl Group, 711
Grigoras, S.
—; Lane, T. H.: Molecular Mechanics Parameters for Organosilicon Compounds Calculated from *Ab Initio* Computations, 136(C)
Guest, M. F. See Price, S. L., 552

Häfelinger, C.
—; Regelmann, C. U.; Krygowski, T. M.; Wozniak, K.: Basis Set Dependence, Precision, and Accuracy of Full *Ab Initio* Gradient Optimizations of Molecular Structures of Nonstrained Hydrocarbons. I. CC Bond Lengths, 329
Harrison, R. J. See Price, S. L., 552
Häser, M.
—; Ahlrichs, R.: Improvements on the Direct SCF Method, 104
Higo, J.
—; Gō, N.: Algorithm for Rapid Calculation of Excluded Volume of Large Molecules, 376
Hinde, R. J. See Miller, K. J., 63
Hosoya, H.
—; Balasubramanian, K.: Computational Algorithms for Matching Polynomials of Graphs from the Characteristic Polynomials of Edge-Weighted Graphs, 698
—; See Randić, M., 683
Howlin, B. See Saldanha, J. W., 975
Huzinaga, S. See Dingle, T. W., 753

Ishida, M. See Takeuchi, K., 380

Jain, D. C.
—; de Gale, D.; Sapse, A.-M.: A Theoretical Study of Solvation Energies of FCH_2COO^-, FCH_2COOH, and F_2CHCOO^-, 1031
Jordan, M. J.
—; Gready, J. E.: Guanidinium-Type Resonance Stabilization and Its Biological Implications. 2. The Doubly-Extended-Guanidine Series, 186
Jug, K.
—; Fasold, E.; Gopinathan, M. S.: A Concept of Charge and Valence for *Ab Initio* Wave Functions, 965

Kalcher, J. See Sax, A. F., 309
Karfunkel, H. R.
—; Eyraud, V.: An Algorithm for the Representation and

Computation of Supermolecular Surfaces and Volumes, 628
Kaufmann, E.
—; von Ragué Schleyer, P.: Degenerate Lithium-Hydrogen Exchange Reactions: *Ab Initio* Models for Metallation Mechanisms Involving H_2, CH_4, NH_3, H_2O, and HF, 437
Kikuchi, T.
—; Némethy, G.; Scheraga, H. A.: Spatial Geometric Arrangements of Disulfide-Crosslinked Loops in Nonplanar Proteins, 287
Klobukowski, M. See Dingle, T. W., 753
Kobeissi, H.
—; Dagher, M.; El-Hajj, A.; Kobeissi, M.: On the Computation of Matrix Elements between Numerical Wave Functions: The Canonical Functions Method, 358
Kobeissi, M. See Kobeissi, H., 358
Krygowski, T. M. See Häfelinger, G., 329
Kuroda, C. See Takeuchi, K., 380

Labanowski, J. K.
—; Dammkoehler, R. A.; Motoc, I.: Orbital Electronegativity and Analytical Representation of Atom Valence State Energy, 1016
Lambert, M. H.
—; Scheraga, H. A.: Pattern Recognition in the Prediction of Protein Structure. I. Tripeptide Conformational Probabilities Calculated from the Amino Acid Sequence, 770
—; Scheraga, H. A.: Pattern Recognition in the Prediction of Protein Structure. II. Chain Conformation from a Probability-Directed Search Procedure, 798
—; Scheraga, H. A.: Pattern Recognition in the Prediction of Protein Structure. III. An Importance-Sampling Minimization Procedure, 817
Lane, T. H. See Grigoras, S., 136(C)
Largo-Cabrerizo, J. See Redondo, P., 295
Lee, I. See Choi, J. Y., 163
Lee, Y. S.
—; Baeck, K. K.; McLean, A. D.: Basis Set Selections for Relativistic Self-Consistent Field Calculations, 112
Lenstra, A. T. H. See Van Alsenoy, C., 302
Lewis, D. F. V.
The Calculation of Molar Polarizabilities by the CNDO/2 Method: Correlation with the Hydrophobic Parameter, Log P, 145
Lii, J.-H.
—; Gallion, S.; Bender, C.; Wikström, H.; Allinger, N. L.; Flurchick, K. M.; Teeter, M. M.: Molecular Mechanics (MM2) Calculations on Peptides and on the Protein Crambin Using the Cyber 205, 503
—; See Tai, J. C., 635
Lindh, R.
—; Malmquist, P.-Å: A Submatrix Algorithm for the Matrix-Vector Multiplication of Very Large Matrices, 344
Lipkowitz, K. B.
—; Baker, B.; Zegarra, R.: Theoretical Studies in Molecular Recognition: Enantioselectivity in Chiral Chromatography, 718
—; Zegarra, R.: Theoretical Studies in Molecular Recognition: Rebek's Cleft, 595
Liu, X.
—; Balasubramanian, K.: Computer Generation of Edge Groups and Edge Colorings, 1
Liu, X
—; Balasubramanian, K.: Computer Generation of the Character Tables of the Symmetric Group (S_n), 417
Lopez, J. P.
Stationary Points on the Potential Energy Surface of O_2^- HF and O_2^- H_2O, 55
López, R. See Rico, J. F., 869

Malmquist, P.-Å. See Lindh, R., 344
Mareda, J. See Müller, P., 863
Martin, J. M. L.
—; François, J. P.; Gijbels, R.: *Ab Initio* Study of the Proton Affinity of a Number of Ortho-Substituted Pyridines, 346
—; François, J. P.; Gijbels, R.: Combined Bond-Polarization Basis Sets for Accurate Determination of Dissociation Energies. II. Basis Set Superposition Error as a Function of the Parent Basis Set, 875
—; François, J. P.; Gijbels, R.: Combined Bond Polarization Function Basis Sets for Accurate *Ab Initio* Calculation of the Dissociation Energies of AH_n Molecules (A = Li to F), 152
—; See Voets, R., 449
Masek, B. B. See Waldman, M., 856
McCammon, J. A. See Davis, M. E., 386
McLean, A. D. See Lee, Y. S., 112
Miller, K. J.
—; Hinde, R. J.; Anderson, J.: First and Second Derivative Matrix Elements for the Stretching, Bending, and Torsional Energy, 63
Moore, K. D. See Chesnut, D. B., 648
Mora, F. See Esteban, A. L., 887
Mosquera, R. A. See Carballeira, L., 911
Motoc, I. See Labanowski, J. K., 1016
Mullens, J. See Voets, R., 449
Müller, P.
—; Mareda, J.: Steric Effects on Reaction Rates. XI. Solvolysis of Tertiary Carbon Substrates Rationalized by Molecular Mechanics Calculations, 863
Murata, Y. See Sotomatsu, T., 94

Némethy, G. See Kikuchi, T., 287

Olefirowicz, E. M.
—; Eliel, E. L.: Conformational Analysis. 48. A Molecular Mechanics (MMP2) Approach to the Conformational Analysis of Methyl-, Dimethyl- and Trimethylisochromanes, 407
Ott, J. J. See Gimarc B. M., 14

Palmer, R. A. See Saldanha, J. W., 975
Polansky, O. E. See Randić, M., 683
Price, S. L.
—; Harrison, R. J.; Guest, M. F.: An *Ab Initio*

Distributed Multipole Study of the Electrostatic Potential Around an Undecapeptide Cyclosporin Derivative and a Comparison with Point Charge Electrostatic Models, 552
Profeta, S., Jr. See Cho, S. G., 832
—; Unwalla, R. J.; Cartledge, F. K.: Simple Alkyldisilanes: MM2 and *Ab Initio* Studies of Their Structures and Barriers to Rotation, 99
Pulay, P. See Zhou, X.-F., 935

Raber, D. J. See Ferguson, D. M., 903
Ramírez, G. See Rico, J. F., 869
Randić, M.
—; Hosoya, H.; Polansky, O. E.: On the Construction of the Matching Polynomial for Unbranched Catacondensed Benzenoids, 683
Redondo, P.
—; Flores, J. R.; Largo-Cabrerizo, J.: Multiple Solutions of Unrestricted Hartree-Fock Equations: The SNH^+ Radical as an Example, 295
Regelmann, C. U. See Häfelinger, G., 329
Rico, J. F.
—; López, R.; Ramírez, G.: Improved Algorithm for the Calculation of One-Electron Two-Center Integrals with STOs, 869
Rios, M. A. See Carballeira, L., 911
Rullmann, J. A. C. See Bellido, M. N., 479

Sabio, M.
—; Topiol, S.: 3*s*- Versus 1*s*-Type Gaussian Primitives: Modifications of the 3-21G(*) Basis Set for the Sulfur Atom, 660
Saldanha, J. W.
—; Howlin, B.; Du Toit, L.; Palmer, R. A.: The Dynamics of Gallimine: A Potent Neuromuscular Blocker. A Determination by Quantum Mechanics and Molecular Dynamics (I) *In Vacuo* Studies, 975
San Fabian, J. See Esteban, A. L., 887
Sánchez-Cabezudo, M. See Catalán, J., 426
Sapse, A.-M. See Jain, D. C., 1031
Saunders, M.
Stochastic Search for the Conformations of Bicyclic Hydrocarbons, 203
Sax, A. F.
—; Kalcher, J.: MC-SCF and CI Calculations on the Si_4H_4 System, 309
Scheraga, H. A. See Kikuchi, T., 287
—; See Lambert, M. H., 770, 798, 817
Schleifer, L. See Aped, P., 265
Schlick, T.
A Recipe for Evaluating and Differentiating $\cos\phi$ Expressions, 951
Sheils, K. See Fărcaşiu, D., 520
Silver, G. L.
Bivariate Interpolation for Experimental Designs, 1013
Smith, C. T. See Ford, G. P., 568
Sotomatsu, T.
—; Murata, Y.; Fujita, T.: Correlation Analysis of Substituent Effects on the Acidity of Benzoic Acids by the AM1 Method, 94
Stewart, J. J. P.
Optimization of Parameters for Semiempirical Methods I. Method, 209
—; Optimization of Parameters for Semiempirical Methods II. Applications, 221
Streitwieser, A. See Bachrach, S. M., 514

Taft, R. W. See Catalán, J., 426
Tai, J. C.
—; Lii, J.-H.; Allinger, N. L.: A Molecular Mechanics (MM2) Study of Furan, Thiophene, and Related Compounds, 635
Takeuchi, K.
—; Kuroda, C.; Ishida, M.: Prolog Program for Subgraph Enumeration and Calculation of Molecular Connectivity Indexes, 380
Teeter, M. M. See Lii, J.-H., 503
Tomasi, J. See Floris, F., 616
Topiol, S. See Sabio, M., 660

Unwalla, R. J. See Cho, S. G., 832
—; See Profeta, S., Jr., 99
Urry, D. W. See Chang, D. K., 850

Van Alsenoy, C.
—; Lenstra, A. T. H.; Geise, H. J.: The Gradient-Optimized Geometry of Haloperidol at the 4-21G Level, 302
Van Opdenbosch, N. See Clark, M., 982
Van Poucke, L. C. See Voets, R., 449
Venanzi, C. A.
—; Canzius, P. M.; Zhang, Z.; Bunce, J. D.: A Molecular Mechanics Analysis of Molecular Recognition by Cyclodextrin Mimics of α-Chymotrypsin, 1038
Voets, R.
—; François, J.-P.; Martin, J. M. L.; Mullens, J.; Yperman, J.; Van Poucke, L. C.: Theoretical Study of the Proton Affinities of 2-, 3-, and 4-Monosubstituted Pyridines in the Gas Phase by Means of MINDO/3, MNDO, and AM1, 449
von Ragué Schleyer, P. See Kaufmann, E., 437

Waldman, M.
—; Masek, B. B.: Analytical Energy Derivatives and Normal Modes in Force Fields Employing Lone-Pair Pseudoatoms, 856
Walter, P. See Fărcaşiu, D., 520
Wang, L.-C. See Boyd, R. J., 367
Wikström, H. See Lii, J.-H., 503
Williams, M. L.
—; Gready J. E.: Guanidinium-Type Resonance Stabilization and Its Biological Implications. I. The Guanidine and Extended-Guanidine Series, 35
Wolfe, S. See Aped, P., 265
Wozniak, K. See Häfelinger, G., 329

Yáñez, M. See Alcamí, M., 468
Yip, V.
—; Elber, R.: Calculations of a List of Neighbors in Molecular Dynamics Simulations, 921
Yperman, J. See Voets, R., 449

Zegarra, R. See Lipkowitz, K. B., 595, 718
Zhang, Z. See Venanzi, C. A., 1038
Zhou, X.-F.
—; Pulay, P.: Characters for Symmetric and Antisymmetric Higher Powers of Representations: Application to the Number of Anharmonic Force Constants in Symmetrical Molecules, 935

Subject Index to Volume 10

Ab initio calculations, atomic charges in, 118
Ab initio calculations, charge and valence in, 965
Ab initio calculations, combined bond-polarization basis sets in, 875
Ab initio calculations, computational improvements in, 104
Ab initio calculations, *d* functions on sulfur, 660
Ab initio calculations, electron correlation effect, 367
Ab initio calculations, for metallation mechanisms, 437
Ab initio calculations, Gaussian basis sets for, 753
Ab initio calculations, improved algorithm for two-center integrals, 869
Ab initio calculations, multiplication of large matrices, 344
Ab initio calculations, of bond lengths in hydrocarbons, 329
Ab initio calculations, of electrostatic potential around an undecapeptide, 552
Ab initio calculations, of nitrogen inversion barriers, 468
Ab initio calculations, of NMR chemical shifts, 648
Ab initio calculations, of polypeptide charges, 479
Ab initio calculations, on carboranes, 14
Ab initio calculations, on complexes of ammonia with hydrides, 603
Ab initio calculations, on disilanes, 99
Ab initio calculations, on dissociation of (A-Li to F) AH_n molecules, 152
Ab initio calculations, on guanidine, 35
Ab initio calculations, on guanidinium-type resonance, 186
Ab initio calculations, on haloperidol, 302
Ab initio calculations, on phosphines and related compounds, 392
Ab initio calculations, on proton affinities in pyridines, 346
Ab initio calculations, on pyrazole and triazole tautomerism, 426
Ab initio calculations, on second row transition metal atoms, 495
Ab initio calculations, on tetrasilatetrahedrane, 309
Ab initio calculations, on the potential surfaces of O_2^- HF and O_2^- H_2O, 55
Ab initio calculations, on the solvation of fluoracetic acid, 1031
Ab initio calculations, population methods in, 514
Ab initio calculations, relativistic, 112
Ab initio calculations, symmetry in, 957
Ab initio calculations, unrestricted Hartree-Fock, 295
Alkanes, linear, conformers of, 520
Ammonia, complexes with hydrides, *ab initio* calculations on, 603
Anomeric effect, $N-C-N$ systems in molecular mechanics, 265
Atomic charges, 118

Basis set superposition error, 875
Benzene, cubic and quartic force constants, 935
Benzenoids, catacondensed, matching polynomial for, 683
Binding site models, using Voronoi polyhedra, 673
Bivariate interpolation, 1013

Canonical functions method, 358
Carbenium ions, molecular mechanics calculations on, 863
Carboranes, *ab initio* calculations on, 14
Character tables, for S_n groups, 417
Charge and valence, in *ab initio* calculations, 965
Chlorosilanes, molecular mechanics calculations on, 832
Cluster method, 928
CNDO calculations. See Semiempirical calculations
Conformers, of linear alkanes, 520
Connectivity indexes, prolog program for subgraph enumeration, 380
Coupled cluster method, for HF, H_2O and NH_3, 928
Coupling constants, in NMR, 887
Crambin, molecular mechanics calculations on, 503
Cyclodextrin mimics, of chymotrypsin, molecular mechanics, 1038
Cyclononane, molecular mechanics calculations on, 903
Cyclosporin, electrostatic potential of, 552

Diatomic molecules, first-row, *ab initio* calculations on, 753
Diffusion quantum Monte Carlo methods, 176
Disilanes, molecular mechanics and *ab initio* calculations on, 99
Dispersion energy, contribution to solvation energy, 616
Dissociation energies of AH_n molecules (A-Li to F), by *ab initio*, 152
Distance geometry, 896
DNA, structure of, 529

Edge groups, of graphs, 1
Edge-weighted graphs, 698
Elastin, molecular dynamics of, 850
Electron correlation, coupled, 928
Electron correlation, in *ab initio* calculations, 367
Electrostatic charges, 118
Electrostatic potentials, by relaxation and conjugate-gradient methods, 386
Enantioselectivity in chiral chromatography, 718

Fluoracetic acid, solvation of, 1031
Force fields, anharmonic, 935

Gallimine, semiempirical and molecular dynamics calculations on, 975
Geometry optimization, derivative evaluation for, 951
Geometry optimization, in semi-empirical calculations, 939
Graph theory, edge groups and edge colorings, 1
Graph theory, for catacondensed benzenoids, 683
Graph theory, matching polynomials, 698
Guanidine, *ab initio* calculations on, 35
Guanidinium-type resonance stabilization, by *ab initio* calculations, 186

Haloperidol, *ab initio* calculations on, 302
Hartree-Fock method, improvements on, 104
Heterocycles, molecular mechanics, calculations on, 635
Hydrocarbons, bond lengths in, by *ab initio* calculations, 329
Hydrophobicity, from semiempirical calculations, 145

Integrals, two-center, improved algorithm for, 869
Ion properties, 367
Isochromanes, molecular mechanics calculations on, 407

Linearized embedding, 896

Matrix multiplication, of very large matrices, 344
Molecular dynamics, of elastin, 850
Molecular dynamics calculations, neighbors list in, 921
Molecular dynamics calculations, on gallimine, 975
Molecular mechanics, enantioselectivity in, 718
Molecular mechanics, first and second derivative matrix elements, 63
Molecular mechanics, for organosilicon compounds, erratum, 136
Molecular mechanics, on cyclodextrin mimics of chymotrypsin, 1038
Molecular mechanics, stochastic conformational space search method, 203
Molecular mechanics, substrate-receptor complexes, 595
Molecular mechanics, the $N-C-N$ anomeric effect, 265
Molecular mechanics, with the 4-fluorophenyl group, 711
Molecular mechanics calculations, Crambin and peptides, 503
Molecular mechanics calculations, Fourier-series expansion of torsional energies, 733
Molecular mechanics calculations, normal modes with lone-pair pseudoatoms, 856
Molecular mechanics calculations, on alkyldisilanes, 99
Molecular mechanics calculations, on carbenium ions, 863
Molecular mechanics calculations, on chlorosilanes, 832
Molecular mechanics calculations, on conjugated oxygen and sulfur heterocycles, 635
Molecular mechanics calculations, on isochromanes, 407
Molecular mechanics calculations, on peroxides, 911
Molecular mechanics calculations, sybyl force field, 982
Molecular mechanics calculations on cyclononane, 903
Molecular mechanics/dynamics, derivative evaluation in, 951
Molecular volume, of a large molecule, 376
Monte Carlo calculations, in diffusion quantum calculations, 176
Monte Carlo calculations, on pentapeptide conformations, 488
Monte Carlo methods, for potential energy surface searching, 203

Neighbors list, in molecular dynamics, 921
Nitrogen inversion barriers, *ab initio* calculations of, 468
NMR, long-range proton-proton coupling constants, 887
NMR chemical shifts, by *ab initio* calculations, 648
Numerov method, convergence of, 413

Orbital electronegativity, analytical representation of, 1016
Organoperoxides, molecular mechanics calculations on, 911

Pattern recognition in, protein structure, 770
Pattern recognition in protein structure, 798, 817
Peptides, conformations of, by Monte Carlo calculations, 488
Peptides, electrostatic potentials around, by *ab initio* calculations, 552
Peptides, molecular mechanics calculations on, 503
Phosphines, and related compounds, *ab initio* calculations on, 392
Point groups, S_n, character tables for, 417
Poisson-Boltzmann equation, solution of, 386
Polarizabilities, by CNDO calculations, 145
Polypeptides, charges in, by *ab initio* calculations, 479
Population methods, in *ab initio* calculations, 514
Potential energy surface searching, in molecular mechanics, 203
Protein structure, in importance-sampling, 817
Protein structure, pattern recognition in, 770
Protein structure, probability-directed search procedure in, 798
Proteins, structural classification of, 287
Proton affinities, *ab initio* calculations on pyridines, 346
Proton affinities of pyridines, semiempirical calculations on, 449
Proton transfer, in water, by AM1 calculations, 163
Pyridines, *ab initio* calculations of proton affinities of, 346
Pyridines, semiempirical calculations of proton affinities of, 449

Quantum Chemistry Literature Database, 748
QSAR, acidity of benzoic acids calculated by AM1, 94

Reaction field theory, 77
Rebek's cleft, molecular mechanics calculations on, 595
Relativistic *ab initio* calculations, 112

Self consistent field method, improvements on, 104
Semiempirical calculations, AM1 on the acidity of benzoic acids, 94
Semiempirical calculations, CNDO calculation of molar polarizabilities, 145
Semiempirical calculations, deorthogonalization of atomic orbitals in, 17
Semiempirical calculations, of proton affinities of pyridines, 449
Semiempirical calculations, of proton transfer in water, 163
Semiempirical calculations, on gallimine, 975
Semiempirical calculations, on reactions of protonated oxirane derivatives, 568
Semiempirical calculations, structure optimization in, 939
Semiempirical methods, parameter optimization, 209, 221
S matrix convergence of, 413
Solvation, from the Lorentz-Debye continuum field, 77
Solvation energies, of fluoroacetic acid, 1031
Solvation energy, dispersion contribution in, 616
Structure, in importance-sampling, 817
Subgraph enumeration, of molecular connectivity, program for, 380
Sulfur, *d* functions on, in *ab initio calculations*, 660
Surface area, of a supermolecule, 628
Sybyl force field program, 982
Symmetry in *ab initio* calculations, 957

Tautomerism, of pyrazole and triazole compounds, 426
Tetrasilatetrahedrane, *ab initio* calculations on, 309
Torsional energies, Fourier-series expansion of, 733
Transition metal atoms, *ab initio* calculations on, 495

Valence state energy, analytical representation of, 1016
Volume, excluded, for large molecules, 376
Volume, of a supermolecule, 628
Voronoi polyhedra, for binding calculations, 673

Wave functions, numerical, matrix elements between, 358